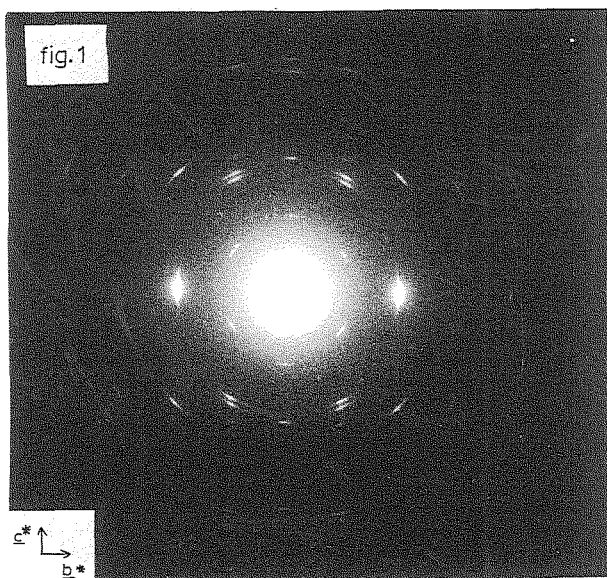


10.2-3 ELECTRON CRYSTAL STRUCTURE ANALYSIS-EPI TAXIALLY GROWN POLYETHYLENE. By Barbara Moss and Douglas L. Dorset, Medical Foundation of Buffalo, 73 High Street, Buffalo, New York 14203, U.S.A.

Epitaxial crystallization of linear polymers onto various substrates allows the possibility of obtaining electron diffraction patterns from zones other than that obtained from solution-grown specimens, from which reliable structural information can be difficult to obtain (the long projection axis enhances crystal bend effects on Bragg intensities (Cowley, *Acta Cryst.* (1961) 14, 920). Wittmann, Hodge and Lotz (*J. Polymer Sci. Polymer Phys.* (1981), 19, 1837; 1853) have described the epitaxial crystallization of polyethylene on benzoic acid. The PE chain axis is oriented parallel to the substrate surface and the $0kl$ diffraction pattern is obtained. The reflections are rather arced. In addition, lkl and $2kl$ type reflections are also observed due to the twisting of lamellae (Keith and Padden, *J. Polymer Sci.* (1959) 39, 101;123) or tilting of successive stacks of lamellae (Bassett and Hodge, *Proc. R. Soc. London* (1978) A359, 121) (Fig. 1). Microcrystals were examined in a JEOL 100B microscope at 100kV. The patterns were recorded on Kodak DEF-5 X-ray film. The films were scanned with a Joyce-Loebl flat bed densitometer and integrated to give Bragg intensities, from which structure amplitudes were derived: $F=I^{1/2}$. Typically 7 to 9 reflections from other zones were recorded in addition to 6 $0kl$ reflections. Agreement with a kinematic calculation (using coordinates derived from paraffins (Abrahamsson *et al.*, *Progr. Chem. Fats. Other Lipids* (1978) 16, 125) and down weighting reflections not from the $0kl$ zone) gives generally poor agreement. Dynamical scattering is important in these data. This presents difficulties as reflections on the tilt axis (the 020 and 040) will have contributions from crystallites oriented in different projections. Considering only the $0kl$ and lkl zones, the sums of intensities not on the tilt axis were used to estimate the relative importance of the two zones. At 284\AA crystal thickness the $0kl$ reflections have fair agreement ($R=.22$) with the dynamical values, while the lkl data also agree reasonably ($R=.19$) at 300\AA thickness. It is apparent that the present analysis is hampered by the need to alter too many variables for too few data. This is in contrast to previous work on epitaxially crystallized paraffin (*J. Polymer Sci. Polymer Phys.*, submitted). Thin, flat, epitaxial crystals of a more perfect nature are required. Work supported by NSF grant DMR81-16318.



10.2-4 STRUCTURE OF IODIDE ION ARRAYS IN IODINATED NYLON 6 AND THE CHAIN ORIENTATION INDUCED BY IODINE IN NYLON 6 FILMS. By N. S. Murthy, A. B. Szollosi, and J. P. Sibilja, ALLIED CORPORATION, Corporate Technology, Morristown, New Jersey 07960 and S. Krimm, Department of Physics, University of Michigan, Ann Arbor, Michigan 48109.

Nylon 6 exists in at least two well characterized crystalline forms referred to as α and γ . In the α form the polymer has a sheet structure of fully extended antiparallel chains connected by hydrogen bonds. The γ form has a shorter chain length (2_1 helix) and the hydrogen bonds are formed between parallel chains. γ form can be obtained by treating nylon 6 with an aqueous solution of iodine-potassium iodide followed by the removal of iodine. Two species of iodide ions (I_3^- and I_5^-) are found in intermediate iodine-nylon 6 complexes. Orientation of I_5^- arrays along the chain axis and I_3^- perpendicular to the chain axis in uniaxially drawn films and in films with planar orientation suggests that there is an intrinsic relation between the direction of iodide ion arrays and nylon 6 chains. When an unoriented film of nylon 6 in the amorphous or the α form is treated with an aqueous solution of iodine-potassium iodide, the I_3^- chains in the resulting iodine-nylon complex lie in planes parallel to the surface of the film, and I_5^- chains are oriented normal to the surface of the film. The γ form obtained by desorbing the iodine from this complex shows considerable orientation with the nylon chains oriented perpendicular to the plane of the film; this orientation is maintained during the γ - α transition. It is proposed that the iodine induced orientation of the nylon 6 chains is due to the nucleating effects of the iodide ion columns as the iodine diffuses unidirectionally into the film.

10.2-5 CRYSTAL AND MOLECULAR STRUCTURE OF COPPER CYCLOHEXYLENEDIAMINETETRAACETATE TETRAHYDRATE. By A. Fuertes, E. Escrivá, D. Beltran, E. Molins, C. Miravittles, Dep. Química Inorg. Fac. Químicas, Univ. Valencia, and Inst. "Jaime Almera" C.S.I.C., Aptdo. Correos 30.102, Barcelona, Spain.

The structure of the compound $Cu_2(CDTA) \cdot 4H_2O$, where $CDTA^{4-}$ is the anion cyclohexylenediaminetetraacetate ($C_{14}H_{18}N_2O_8^{4-}$), has been determined by X-Ray techniques to clarify the coordination geometry around the two copper atoms and the packing of the complex. Crystals are orthorhombic with $a = 10.863(3)$, $b = 12.074(4)$, $c = 14.802(6)$ Å, $V = 1941.3$ Å³; the space group $P2_12_12_1$, $Z = 4$. Intensity data were collected on a CAD 4 Diffractometer using $MoK\alpha$ radiation.

The structure was solved with the MULTAN 11/82 system (Main, P. et al., 1982). An E-map computed with the phases from the set with the highest combined figure of merit revealed peaks for nine non-hydrogen atoms and the two Cu atoms, the remaining were located with a Fourier Synthesis. The structure was anisotropically refined by means of full matrix least-squares with the SHELX-76 program (Shel-

